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memorandum

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SUBJECT: Cross-section and Reaction Nomenclature for MCNP Continuous-energy Libraries and DANTSYS Multigroup Libraries

There has been much discussion recently on the nomenclature used in specifying reaction (and groups of reactions) cross-sections in MCNP and DANTSYS. Unfortunately, there is no method for making equivalent definitions between MCNP and DANTSYS, but we can make definitions that are somewhat closer in meaning than we have currently. We will first review the definitions that MCNP currently uses, and a proposal to make these somewhat more consistent to DANTSYS. Since it is not possible to have equivalent definitions between the two codes, consideration must be given to the confusion to the users that changing the nomenclature within MCNP would cause versus any small gain that might be made. We will not discuss the MCNP multigroup capability at this time as this would only further confuse the issue.

Continuous-energy libraries in MCNP

Table 1 lists the definitions that are currently used relative to the continuous-energy cross-section data in MCNP. The multiplicity information for individual reactions is given

Table 1: Current MCNP Nomenclature for Continuous-energy Libraries

Nomenclature	Reaction MT Values	Description
Total cross section	MT=1	Sum of all reaction cross sections
Elastic cross section	MT=2	Elastic reaction only
Total Absorption cross section	MT=101=Sum(102-116)	Sum of all reaction cross sections where no neutron is emitted.
Total Fission	MT=18 or Sum(19,20,21,38)	Total fission cross section
By default, MCNP knows, but never uses:		
Non-elastic cross section	MT=3=Total-elastic-absorption-fission	The sum of all reaction cross sections not included in MT’s=2,101,18

in the secondary particle information, and is not part of the cross section. For instance, the (n,2n) reaction is specified by MT=16. The information that two neutrons are emitted by MT=16 is contained in another part of the data library and is not in the cross section information.

Additionally, the (n,γ) reaction is specified by MT=102 and is often referred to as the capture reaction. This term is often misleading for many users as it can be confused with total absorption as defined in Table 1.

One proposal for a more standard terminology is given in Table 2 for continuous-energy data in MCNP. The term “disappearance cross section” would now replace the “absorption cross section”. The new total absorption cross section would include the total fission cross section as well. MCNP would not use this newly defined total absorption cross section, but it could be made available to the user for an FM tally, etc. Other definitions would remain the same.

Table 2: One Proposal for MCNP Nomenclature for Continuous-energy Libraries

Nomenclature	Reaction MT Values	Description
Total cross section	MT=1	Sum of all reaction cross sections
Elastic cross section	MT=2	Elastic reaction only
Disappearance cross section	MT=101=Sum(102-116)	Sum of all reaction cross sections where no neutron is emitted.
Total Fission	MT=18 or Sum(19,20,21,38)	Total fission cross section
Total Absorption cross section	MT=27=Sum(18,101)	Absorption is defined as disappearance plus fission
By default, MCNP knows, but never uses:		
Non-elastic cross section	MT=3=Total-elastic-disappearance-fission =Total-elastic-absorption	The sum of all reaction cross sections not included in MT’s=2,101,18

For both the current and proposed nomenclature, one can construct a total scattering cross section that is equal to the elastic (MT=2) plus non-elastic (MT=3) cross sections.

$$\sigma_{sc}=\sigma_{el}+\sigma_{non\text{-}el} .$$

Note that the non-elastic (MT=3) is <u>not</u> the inelastic cross section (MT=4=Sum(51-90)). The non-elastic cross section includes reactions such as (n,2n), (n,n’α), etc. Furthermore, remember that NONE of the scattering cross sections referred to here include multiplicities. As stated previously, MCNP also has available multiplicity information for each individual reaction. This includes ν(E), the average number of neutrons emitted per fission. On MCNP libraries, most often both prompt and total $\nu(E)$ are available (see Appendix G of the manual). Within MCNP, however, only prompt or total nubar is available (depending on the various entries in the users INP file).

Nomenclature for Multigroup Libraries in DANTSYS

Now, let us try to tie these same proposed terms for continuous-energy libraries in MCNP to multigroup libraries for DANTSYS. Unfortunately, there is no possibility for having equivalent definitions between the two types of libraries. This is because multigroup libraries have available more limited (and different) data than do continuous-energy libraries.

In general, multigroup libraries only have the following data available: $\sigma_{absorption}$, $\nu\sigma_{fission}$, σ_{total}, and scattering matrices. Lets look at each of these types of data and how they relate to continuous-energy quantities.

σ^i_{total} : total cross sections in group i. Usually, this is the ONLY quantity that has a one-to-one correspondence with anything listed in Tables 1 or 2. It clearly corresponds to MT=1. However, if certain transport-correction options are used in DANTSYS, then even the total cross section *will not* strictly have the same meaning as in continuous-energy libraries.

scattering matrices: For this discussion, we need only be concerned with the P0 matrix. We will refer to the element of the P0 matrix that contains the scattering cross section from group i to group j as $\sigma_s^{i\text{->}j}$. Generally, what people refer to as the multigroup scattering cross sections for group i is calculated as

$$\sigma^i_{sc} = \sum_{j=1}^{NG} \sigma_s^{i\to j} ,$$

where NG is the number of groups. What quantity in Table 2 does this correspond to? The answer is <u>none</u>. The reason there is no corresponding quantity is that none of the quantities in Table 2 include multiplicities. Therefore, σ^i_{sc} is most like MT2+MT3, but it is by no means the same quantity.

$\nu\sigma^i_{fission}$: nubar times the fission cross section in group i. This quantity corresponds to the product of MT=18 from Table 1 or 2 and nubar (available to MCNP users via the FM tally with MT=-7). One limitation of multigroup libraries is that $\nu\sigma_f$ represents either prompt or total fission, but never both. The flexibility associated with MCNP continuous-energy libraries is therefore generally unavailable.

$\sigma^i_{absorption}$: the absorption cross section in group i. The first thing to note is that the absorption cross section is totally irrelevant to the DANT solution of the transport equation. The value of σ^i_{abs} is clearly relevant, however, if used as an edit quantity.

The second thing to note is that it is impossible to predict what σ^i_{abs} represents without knowing exactly now the library was produced. It is very possible that σ^i_{abs} on a multigroup library may be equivalent to either MT=101 or MT=27, the disappearance or absorption cross section as defined in Table 2.

Frequently, σ^i_{abs} will be the "particle-balance absorption cross section", defined as

$$\sigma^i_{abs\ part\text{-}bal} = \sigma^i_{total} - \sigma^i_{sc} ,$$

This quantity is very different than MT=27, because of the multiplicities of the individual reactions. Since σ_{sc} includes multiplicities, so does $\sigma_{abs\ part\text{-}bal}$, although in a negative sense. For example, the (n,2n) reaction contributes 2*$\sigma_{n,2n}$ to σ_{sc}. It therefore contributes -1*$\sigma_{n,2n}$ to $\sigma_{abs\ part\text{-}bal}$. $\sigma_{abs\ part\text{-}bal}$ has no counterpart to a quantity in Table 2 or to an actual physical quantity. One further note - even if σ^i_{abs} in a multigroup library does correspond to MT=27, DANTSYS allows the user to replace the library value with a DANT calculated $\sigma_{abs\ part\text{-}bal}$.

Before ending this discussion, we should note that careful generation of a multigroup library can include any quantity one may desire, in the form of edit cross sections. Therefore, any quantity in Table 2, in theory, could be made available on a multigroup library. Since this is not the standard method of multigroup library generation, the conclusion is that even for multigroup and continuous-energy libraries derived from the identical evaluated data, cross section quantities available to DANTSYS and MCNP are very difficult to correlate precisely to one another. Since it is not possible to have equivalent definitions between the two codes, consideration must be given to the confusion to the users that changing the nomenclature within MCNP would cause versus any small gain that might be made.